2-Methylpropionic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C11H11NO2/c1-8(2)11(13)14-10-5-3-9(7-12)4-6-10/h3-6,8H,1-2H3
InchiKey: YCYITKXAJQLLDP-UHFFFAOYSA-N
Formula: C11H11NO2
SMILES: CC(C)C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 189.21

Physical Properties

Property code	Value	Unit	Source
gf	41.34	kJ/mol	Joback Method
hf	-130.51	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.120		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
tb	660.67	K	Joback Method
tc	889.47	K	Joback Method
tf	374.82	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.44	J/mol×K	660.67	Joback Method
cpg	383.28	J/mol×K	698.80	Joback Method
cpg	394.31	J/mol×K	736.94	Joback Method
cpg	404.55	J/mol×K	775.07	Joback Method
cpg	414.02	J/mol×K	813.20	Joback Method
cpg	422.74	J/mol×K	851.34	Joback Method
cpg	430.71	J/mol×K	889.47	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume